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Turbulent Diffusion Behind Vehicles
Evaluation of Roadway Models

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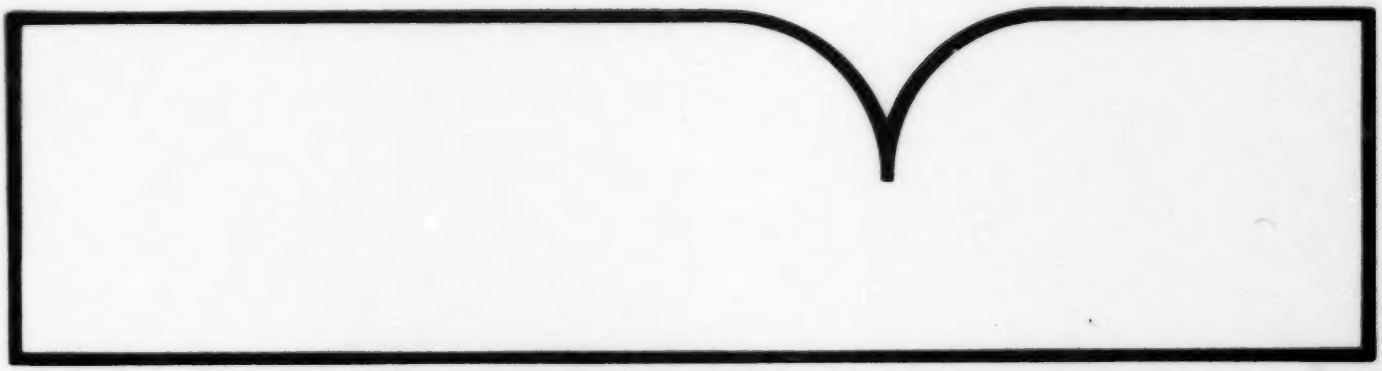

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16. ABSTRACT

This paper presents a statistical evaluation of three highway air pollution models (CALINE 3, HIWAY-2, and ROADWAY) using the tracer data from the General Motors Sulfate Dispersion Experiment. Since the models predict the ensemble mean whereas any given observation reflects a single realization or an event from a population, it should be recognized that the model predictions will almost always differ from the corresponding observations, even if the models and the input data for the models are perfect. The bootstrap resampling procedure is used to quantify the variability in the observed concentrations due to the stochastic nature of the atmosphere. The results suggest that the variability in the observations due to the random nature of the atmosphere is about 30%. Therefore, if the predicted values are within ± 30% of the measured concentrations, the differences between model predictions and observations should not be considered to be significant. Thus a 'perfect' air quality should predict to within ± 30% of its corresponding observed concentrations. Comparisons of the model predictions paired and unpaired in time with measurements suggest that HIWAY-2 and ROADWAY perform best, but the performance of CALINE 3 is acceptable. Application of the extreme value theory and the bootstrap resampling procedure to the modeled and measured data (unpaired) shows that all three models are capable of predicting the extreme concentrations within the model performance criteria set forth above.

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TURBULENT DIFFUSION BEHIND VEHICLES: EVALUATION OF ROADWAY MODELS

S. T. RAO* and G. SISTLA
Division of Air Resources, NYS Dept. of Environmental Conservation, Albany, NY 12233, U.S.A.

and

R. E. ESKRIDGE† and W. B. PETERSEN†
Atmospheric Sciences Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711, U.S.A.

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Abstract—This paper presents a statistical evaluation of three highway air pollution models (CALINE3, HIWAY-2, and ROADWAY) using the tracer data from the General Motors Sulfate Dispersion Experiment. Since the models predict the ensemble mean whereas any given observation reflects a single realization or an event from a population, it should be recognized that the model predictions will almost always differ from the corresponding observations, even if the models and the input data for the models are perfect. The bootstrap resampling procedure is used to quantify the variability in the observed concentrations due to the stochastic nature of the atmosphere. The results suggest that the variability in the observations due to the random nature of the atmosphere is about 30%. Therefore, if the predicted values are within ±30% of the measured concentrations, the differences between model predictions and observations should not be considered to be significant. Thus a 'perfect' air quality model should predict to within ±30% of its corresponding observed concentrations. Comparisons of the model predictions paired and unpaired in time with measurements suggest that HIWAY-2 and ROADWAY perform best, but the performance of CALINE3 is acceptable. Application of the extreme value theory and the bootstrap resampling procedure to the modeled and measured data (unpaired) shows that all three models are capable of predicting the extreme concentrations within the model performance criteria set forth above.

1. INTRODUCTION

The passage of the National Environmental Policy Act of 1969 initiated modeling of pollution due to vehicles. This act requires that for new highways that are partially funded by federal funds an environmental impact statement should be prepared before construction begins. A number of highway air pollution models were developed in the early 1970s such as CALINE (Beaton *et al.*, 1972), EGAMA (Egan *et al.*, 1973), and HIWAY (Zimmerman and Thompson, 1975). Attempts to validate and evaluate these models with experimental data taken near highways were not satisfactory because of the uncertainty in the estimate of the emissions from vehicles. In field experiments the background of measured pollutants was nonhomogeneous. Also, the statistical tests used in previous model evaluations were rather simple. In 1975 General Motors, with the cooperation of Ford Motor Co., the Chrysler Corp. and the U.S. Environmental Protection Agency, conducted a well conceived and controlled highway experiment at the General Motors test facility (Cadle *et al.*, 1976). The tracer data from this experiment furnished for the first time an outstanding data set for model evaluation and development.

The Environmental Protection Agency funded the American Meteorology Society to establish a group of scientists to evaluate and recommend techniques for use in model evaluation. The recommendations of this group are given by Fox (1981). In a response to the recommendations of the American Meteorological Society, Willmott (1982) made a number of important suggestions.

In the late 1970s and early 1980s a number of highway models were developed, and many of these were evaluated by Rao *et al.* (1980) using the General Motors data and many of the techniques recommended by Fox (1981). In this paper three highway models (CALINE3, HIWAY-2 and ROADWAY) will be evaluated using the General Motors tracer data and the statistical techniques suggested by Fox and Willmott, extreme value statistics (Tabony, 1983), and the 'bootstrap' method (Diaconis and Efron, 1983).

2. HIGHWAY MODELS

(a) *The CALINE3 model*

CALINE3 is a line source model developed by the California Department of Transportation (Benson, 1979). It is based on the Gaussian diffusion equation

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†On assignment from NOAA, and to whom correspondence should be addressed.

and employs a mixing zone concept to characterize pollutant diffusion over the roadway. The model divides individual highway sections into a series of elements from which incremental concentrations are computed from an approximation to the crosswind finite line source equation and summed to form a total concentration estimate at a particular receptor location. Each element is modeled as an equivalent finite line source positioned normal to the wind direction and centered at the element midpoint. The region directly over the highway is treated as a zone of uniform emissions and turbulence.

The vertical diffusion parameter is a modification of the curves suggested by Pasquill (1974) to incorporate the initial diffusion over the highway. The horizontal diffusion curves are identical to those suggested by Turner (1970) except for averaging time and surface roughness power law adjustments similar to those made for the vertical diffusion curves.

(b) *The HIWAY-2 model*

The HIWAY-2 model (Rao and Keenan, 1980) is basically a Gaussian diffusion model developed for at grade and cut section roadway configurations. Highway emissions are considered to be equivalent to a series of finite line sources. Each lane of traffic is modeled as if it were a straight, continuous, finite line source with a uniform emission rate. A highway is simulated with an increasing number of point sources with the total contribution of all points computed by a trapezoidal integration of the Gaussian point source equation over a finite length until the solution converges.

The diffusion parameters used in HIWAY-2 were determined from the tracer data collected during the General Motors Experiment and the Long Island Expressway Experiment (Sistla *et al.*, 1979). Downwind diffusion is a function of initial diffusion and stability class. Three stability regimes are utilized to characterize downwind diffusion. The initial spread has incorporated in it a vehicle-induced drag factor that accounts for the initial dilution of the pollutant over the roadway, and allows the model to make reasonable estimates of concentrations when the wind speed is low and the wind direction is parallel to the roadway.

(c) *The ROADWAY model*

The ROADWAY model solves a conservation of species equation via finite-difference approximations. The model assumes a surface layer describable by surface layer similarity theory with the superposition of the effects of vehicle wakes. The vehicle wakes affect the wind field and the turbulence fields, and it is assumed in the model that the effect is linear. The unique part of the ROADWAY model is the vehicle wake theory, which was originally developed by Eskridge and Hunt (1979), and modified by Eskridge and Thompson (1982) and Eskridge and Rao (1983, 1986).

A vehicle wake is a region of increased turbulence and decreased velocity relative to the vehicle. The intensity of the wake is a function of vehicle speed, downwind distance, and distance from the center of the wake. An averaged velocity and turbulence field is calculated across the highway based upon the number of vehicles, vehicle speeds, and ambient, atmospheric (upwind) conditions. Using the calculated velocity and turbulence fields, pollutant concentration predictions are made over, upwind and downwind of the highway. It is worth noting that unlike CALINE3 and HIWAY-2, the ROADWAY model development was independent of the General Motors data.

3. EVALUATION AND COMPARISON OF HIGHWAY POLLUTION MODELS

In this section the performance characteristics of three diffusion models, HIWAY-2, CALINE3 and ROADWAY, will be determined using the data from the General Motors Sulfate Dispersion Experiment. It should be borne in mind that HIWAY-2 and CALINE3 are expected to perform well when tested against the data from which they were developed. Further, it is worth noting that the physics of the problem is handled differently in all three of these models. By making intercomparison of model results it is possible to make an assessment of each model's simulation capability as a function of different treatments of modeling of pollutant transport and diffusion near roadways.

Two techniques are used to compare the predicted and measured concentrations, namely paired and unpaired comparisons. A paired analysis allows a direct comparison of individual predictions with measured values, while unpaired techniques determine model behavior on a statistical basis, without regard to the spatial and temporal correspondence between measured and predicted concentrations. The techniques used in the paired and unpaired analysis are described in Fox (1981) and Rao *et al.* (1985), and the unpaired (bootstrap) is described below. The results from the paired analyses, summarized in Table 1, indicate that HIWAY-2, ROADWAY and CALINE3 explain about 70%, 65% and 29% of the variance, respectively. The slopes of the regression lines are close to unity with small intercept values for all three models. The Index of Agreement, which reflects the degree to which the observation is accurately simulated by the model, shows that HIWAY-2 is 5% better than ROADWAY and both are considerably better than CALINE3. A second strong measure of model performance is the root-mean-square error (RMSE) which indicates the size of the error produced in the model; Table 1 shows that HIWAY-2 and ROADWAY perform considerably better than CALINE3. The mean fractional error shows that CALINE3 tends to underpredict slightly and HIWAY-2 and ROADWAY tend to overpredict. Mean fractional error is not a good measure by itself, as it would

Table 1. Comparison of model results using the GM data

	OBSERVED	HIWAY-2	CALINE3	ROADWAY
Range	0.01–4.92	0.01–4.68	0.09–17.97	0.02–5.29
Mean	0.96	1.07	0.96	1.20
Standard deviation	0.74	0.77	1.31	0.92
R^2		0.70	0.29	0.65
Slope		0.87	0.96	1.00
Intercept		0.23	0.04	0.25
Mean of (P/O)		1.30	1.23	1.40
Standard Deviation of (P/O)		0.99	1.20	1.02
Mean difference (d)		0.11	0.00	0.25
Variance of the difference (S_d^2)		0.18	1.23	0.29
Average absolute gross error $(1d1)$		0.30	0.41	0.41
Root-mean-square error $(RMSE_d)$		0.44	1.11	0.60
Index of agreement (D)		0.91	0.64	0.86
Mean fractional error (MFE)		−0.12	0.04	−0.21
Unsystematic mean square error (MSE_u)		0.18	1.22	0.29
Systematic mean square error (MSE_s)		0.02	0.00	0.06
Mean square error (MSE)		0.20	1.22	0.35
MSE_u/MSE		89%	100%	83%
MSE_s/MSE		11%	0%	17%

$N = 594$.

indicate here that CALINE3 is the best model, but the other statistical tests indicate otherwise. The mean fractional error could be small if there are large overpredictions balanced by large underpredictions. The average errors between predictions and measurements are similar for ROADWAY and HIWAY-2, although the simulation of HIWAY-2 is slightly better than that of ROADWAY. Particularly noteworthy is the fact that the errors of all three models are mostly unsystematic. For a good model the systematic difference should approach zero and the unsystematic difference should approach the root-mean-square error. The fact that similar results are found for both HIWAY-2 and ROADWAY is indicative of the appropriateness of the methodologies utilized in these models, even though they are based on completely different treatments of the physics of the problem. The ROADWAY model uses vehicle wake theory, while HIWAY-2 uses simple parameterizations of traffic-induced turbulence from a Gaussian approach to handle the transport and diffusion of pollutants near roadways.

In the following analysis, account is taken of the fact that the observations include measurement error, as well as the variability due to the stochastic or random nature of the atmosphere. It is imperative that this variability be considered in model evaluation. Any model prediction represents an ensemble average, while any given observation reflects a specific realization from a population that will almost always differ from the prediction, even if the model and the input data are perfect. Thus, it should be recognized that there is no significant difference between model predictions and observations as long as the predictions are contained within the natural variability of the observed concentrations. Assuming that the concentrations are directly proportional to the emission strength and indirectly proportional to the wind speed, the variability in the normalized concentration CU/Q (where C is the tracer gas concentration, U is the wind speed, and Q is the emission strength) can be determined using the General Motors data at the nearest roadside ground level receptor under nearly perpendicular wind–road orientations. Since previous investigations (Eskridge and Rao, 1983; Eskridge *et al.*, 1979; Rao *et al.*, 1979) on the role of traffic-induced turbulence imply the concentrations immediately adjacent to the roadway in the downwind direction are independent of the atmospheric stability, and that pollutant diffusion is dictated by the locally generated turbulence, it is reasonable to combine all data from the nearest roadside ground level (0.5 m height) monitor in the downwind direction to investigate the atmospheric–experimental variability. Furthermore, the data are restricted to the 18 cases with wind direction nearly perpendicular to the roadway, since then the transport and diffusion from the source to the receptor are well defined. The design of the General Motors experiment ensures that the mechanical turbulence generated by the moving vehicles will be approximately the same for all tracer experiments, because of constant vehicle speed as well as spacing of vehicle packs and vehicles in the packs. Thus, the analysis of the normalized concentration CU/Q for all perpendicular wind–road orientation cases allows an estimation of the magnitude of the atmospheric–experimental variability (stochastic process).

The cumulative probability plot of normalized concentration is shown in Fig. 1. The computed mean for CU/Q, the standard deviation of CU/Q, and the coefficient of variation (ratio of the standard deviation to the mean) about the mean are 0.587, 0.154 and 26%, respectively. Thus, the mean for this sample can be reported as $\hat{\rho} = 0.587 \pm 0.154$. This indicates that the best guess of the unknown true value ρ is $\hat{\rho} = 0.587$,

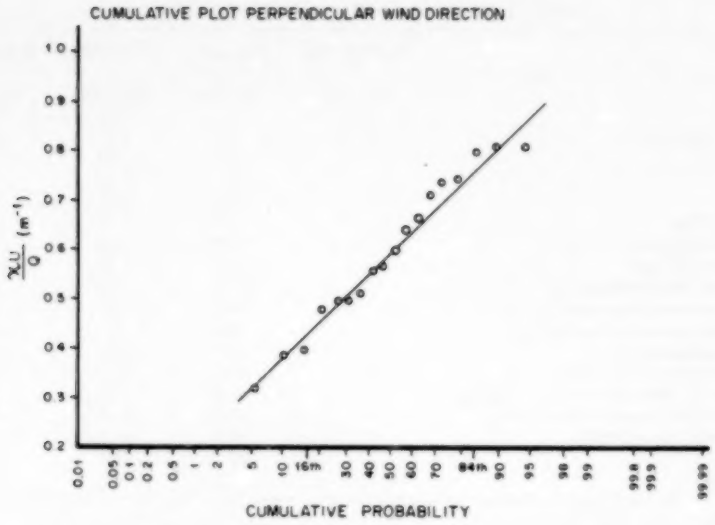

Fig. 1. Cumulative frequency distribution of the normalized concentrations at the nearest roadside receptor under perpendicular wind–road orientation.

with an expected root-mean-square error of 0.154 for $(\rho - \hat{\rho})$. If $(\rho - \hat{\rho})$ has roughly a normal distribution (this may always be the case for large data sets), then the accuracy statement can be interpreted as PROB $\{\rho \varepsilon [0.587 - 0.154, 0.587 + 0.154]\} = 0.68$. The above statement is based upon the fact that for a normal distribution, 68% of the data are within one standard deviation of the mean. The accuracy of the estimated mean value can be assessed using the 'bootstrap' method (see Diaconis and Efron (1983) for a detailed description of the method) which is as follows:

(a) Let F be the set of the observed data points (18 in this analysis).

(b) Use a random number generator to draw a set of 18 points independently from F, so that each member of the set is an independent random selection of one of the 18 original data points. This new data set, called the bootstrap sample, is a subset of the original set, which is plotted in Fig. 1. Some of the original points will have been selected zero times, some once, some twice, etc.

(c) Compute the mean $(\hat{\rho}^*)$, the standard deviation $(\hat{\sigma}^*)$, and the coefficient of variation $(\hat{\theta}^*)$ of the bootstrap set.

(d) Repeat steps (b) and (c) above, a large number of times, say N ($N = 1000$ here), each time using an independent set of new random numbers to generate the bootstrap set. Denote the resulting sequence of bootstrap means by $\hat{\rho}^{*1}, \hat{\rho}^{*2}, \ldots, \hat{\rho}^{*N}$.

(e) Construct a histogram plot of $(\hat{\rho}^{*1} - \hat{\rho})$, $(\hat{\rho}^{*2} - \hat{\rho}), \ldots, (\hat{\rho}^{*N} - \hat{\rho})$ based on the N bootstrap sets (called replications).

The histograms based on the 1000 bootstrap replications of the mean of the sample, the standard deviation, and the coefficient of variation are plotted in Fig. 2. The coefficient of variation from the bootstrap replications was found to vary as much as 5% from the estimate based on the original sample (26%). Thus, the overall variation in the original sample will be *approximately* 30%. This limit of plus or minus 30% of the observed normalized concentrations represents the variability in the observed concentration due to the stochastic nature of the atmosphere and should be taken into account in model evaluation studies. Figure 3 shows a scatter plot of observed concentrations, under near perpendicular cases for the GM data, and the predicted concentrations from the HIWAY-2, CALINE3 and ROADWAY models for the data set used in the bootstrap analysis. From the scatter plot, it is observed that 64% of the data points from the three models are within the natural variability. There is a bias towards over predicting in the three models. The models cannot be expected to perform better than plus or minus 30% of the observed concentrations. Table 2 shows how each model performed with the GM data in predicting the maximum concentrations for each tracer experiment, as well as for the entire data set taken downwind of the road. Again, it is worth noting the similarity of performance between the HIWAY-2 and ROADWAY models in predicting the maximum concentrations. When the entire data set is considered, HIWAY-2 and ROADWAY performed somewhat better than CALINE3, but all have an acceptable level of performance. Table 2 shows that when all data are considered the models perform about the same. Included in Table 2 are the results from the HIWAY model to facilitate a comparison among the models and to document the improvement over the HIWAY model.

While the three models perform well in terms of the GM data base as a whole, their ability to predict high

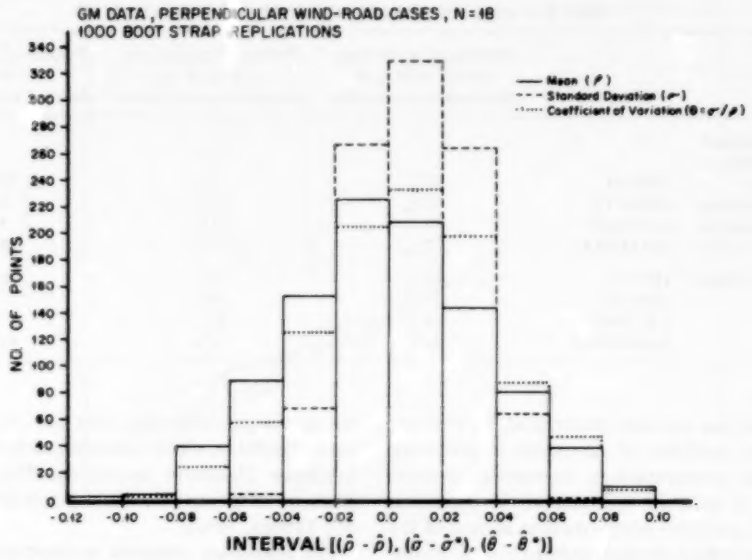
GM DATA, PERPENDICULAR WIND-ROAD CASES, N=18
1000 BOOT STRAP REPLICATIONS
Mean ($\hat{\rho}$)
Standard Deviation ($\hat{\sigma}$)
Coefficient of Variation ($\theta = \sigma/\rho$)
NO. OF POINTS
INTERVAL [($\hat{\rho}$ - $\hat{\rho}$), ($\hat{\sigma}$ - $\hat{\sigma}^*$), ($\hat{\theta}$ - $\hat{\theta}^*$)]

Fig. 2. Uncertainty distribution for the selected parameters using 1000 bootstrap replications.

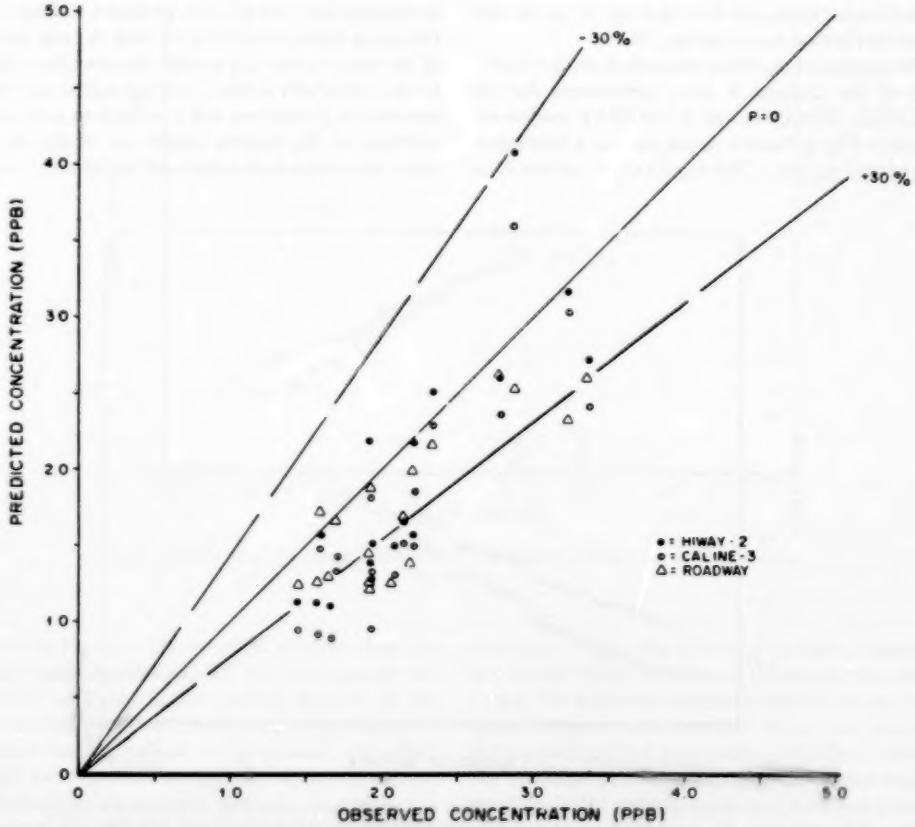

Fig. 3. Scatter plot of model predictions and measurements.

Table 3. Model comparison of second highest concentration (ppb)

Model	Mode	Sample size	Predicted $	Observed	Boot strap 95% confidence interval
HIWAY-2	1.839	61	4.219 ± 1.057	3.770	3.40–4.37
CALINE3	1.525	60*	4.207 ± 1.191	3.770	3.10–4.80
ROADWAY	1.895	61	4.665 ± 1.230	3.770	3.56–4.69

95% confidence limit to the model predicted second highest concentration based on the extreme value distribution.
*One tracer run with very low wind speed is removed from this analysis.

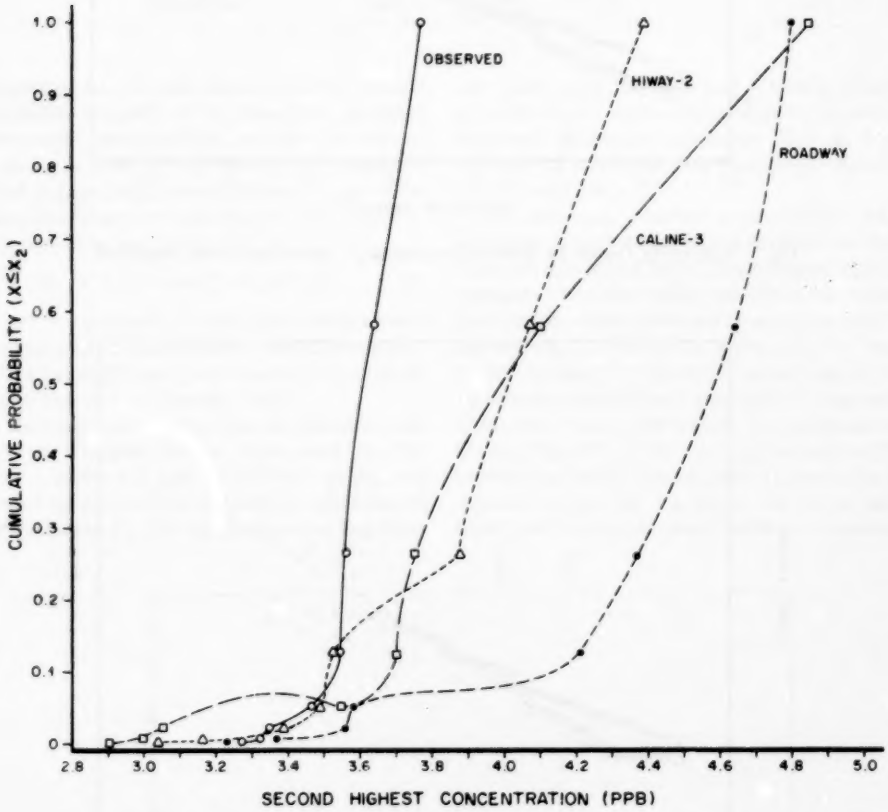

Fig. 7. Cumulative frequency distribution of model-based and the observation-based second highest concentration using 1000 bootstrap replications.

tration than that measured for a given probability. The ROADWAY model provides a more conservative estimate (i.e. higher) of the concentration than the other models. At 50% probability, the observed data indicate that the second highest of the maximum concentration is 3.62 ppb, while for the ROADWAY model it is 4.58 ppb. Given that there is no significant difference between model predictions and measurements as long as the predictions are contained within plus or minus 30% of the measured concentrations, the above result indicates that the predictions from the ROADWAY model, as well as the other two models, are in agreement with the measurements. Thus, these models are seen to provide slightly conservative and realistic estimates of the concentrations. Not only the central tendencies, but also the extreme values produced by these models (especially HIWAY-2 and ROADWAY) are observed to be in good agreement with the measured data.

4. SUMMARY

The performance of CALINE3, HIWAY-2 and ROADWAY has been assessed using the tracer data

from the General Motors Sulfate Dispersion Experiment. The model predictions were first paired in time with the observations and various statistical parameters were evaluated. These tests indicate all three models perform well with the General Motors data, but HIWAY-2 and ROADWAY simulate the data better than CALINE3.

Using the bootstrap method and the normalized observations immediately downwind of the road, it was shown that there is an expected variation in the data of about $\pm 30\%$. This variability in the observed concentrations is due to measurement errors and the randomness of the atmosphere. The implication of this natural variability is that model predictions within $\pm 30\%$ of the observations can not be improved upon with this data set.

To test how well the models predict extreme values, asymptotic extreme value theory and the bootstrap method were used. The results indicate that all three models performed well in predicting the extreme concentrations.

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